An Implicit "Drift-Lorentz" Mover for Plasma and Beam Simulations

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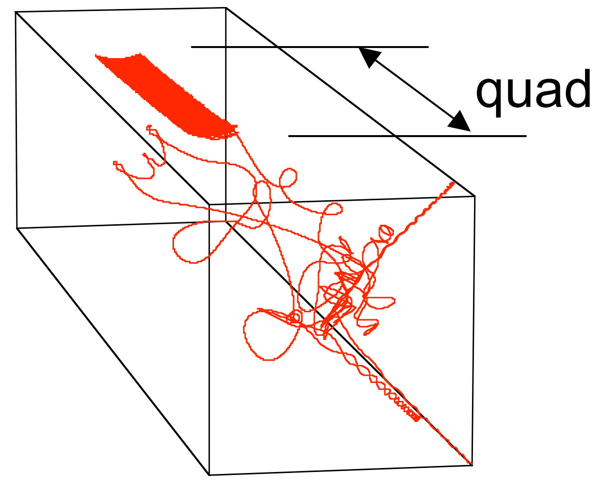
OUTLINE

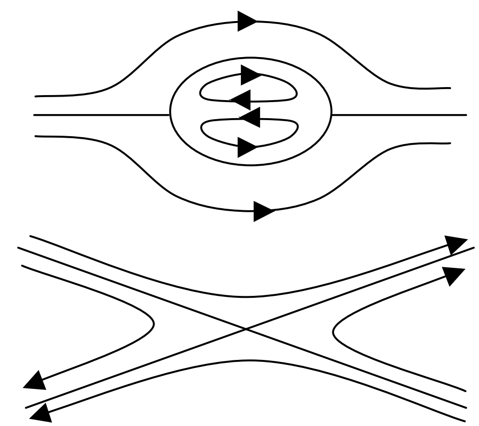
- Motivation
- The basic blended mover
- Previous step toward implicitness (HIF ’06)
- The new algorithm
- Tests
  - Orbits
  - Buneman Instability
  - Fast faraday cup plasma
- Conclusions

Our initial motivation was simulation of electron clouds in quadrupole-focussed HIF accelerators…

- e-clouds are a major concern for HIF (and other pos.-charge) accelerators
- Computational challenge
  - Electrons strongly magnetized in quads
  - Unmagnetized near nulls and between magnets
  - Need to follow electrons through both regions



- Other examples:
  - Systems with B-field nulls (MFE field-reversed conigurations, bow shock, other systems with magnetic reconnection)
  - Systems with localized strong B fields ("Picket-fence" magnetic configurations, high-order multipoles, Localized self-generated B fields)



Our basic approach blends full-particle dynamics and drift kinetics

- Historical inspiration: Parker & Birdsall (JCP '91)
  - showed that standard Boris mover at large $\omega_c \Delta t$ produces correct **E**x**B** and magnetic drifts
  - Price: anomalously large "gyro" radius ($\sim \rho\ \omega_c \Delta t$) and anomalously low "gyro" frequency
  - For our applications, low "gyro" freq. OK but large "gyroradius" is not
- Our solution: interpolate between full-particle dynamics (Boris mover) and drift kinetics (motion along B plus drifts).

The basic procedure is simple… (Ref: R. Cohen et al, Phys. Plasmas **12**, 056708 (2005).

- Update instantaneous velocities

$$\mathbf{v}_{L,new} = \mathbf{v}_{L,old} + \left[(\Delta \mathbf{v})_{Lorentz} + (1-\alpha)\,(\Delta \mathbf{v})_{\mu \nabla B} \right]$$

  – Last term is mirror-force correction term (see below)

- Update particles using blend of this velocity and drift velocity:

$$\mathbf{v}_{eff} = \mathbf{b}(\mathbf{b}\cdot\mathbf{v}_L) + \alpha \mathbf{v}_{L,\perp} + (1-\alpha)\mathbf{v}_d$$

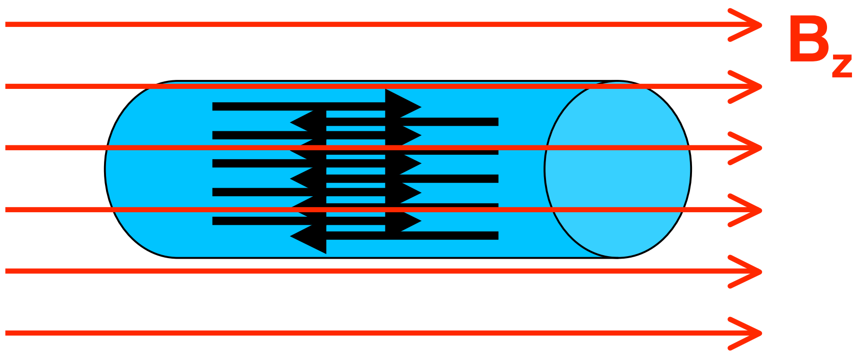
  – Here α is an interpolation constant. The particular choice

$$\alpha = 1/[1+(\omega_c \delta t/2)^2]^{1/2}$$

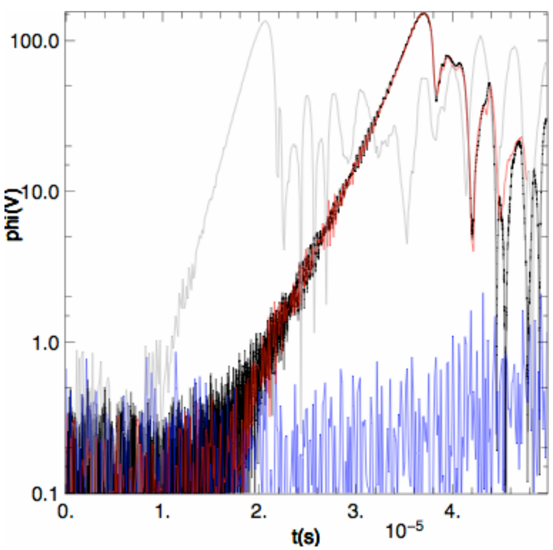
  preserves the physically correct gyroradius at large $\omega_c \Delta t$

- The term $\Delta v_{\mu\nabla B}$ is the "magnetic mirror force" which arises from the convergence or divergence of field lines. It is properly calculated in full particle dynamics but needs to be explicitly added to drift kinetics. Hence the $(1-\alpha)$ multiplier.
  – Can represent as rotation by $\Delta\theta = (m\mu/2B^3)^{1/2}\Delta t \mathbf{B}\cdot\nabla B$ in plane defined by $\mathbf{v}_L$ and $\mathbf{B}$, where $\mu = mv_\perp^2/2B$

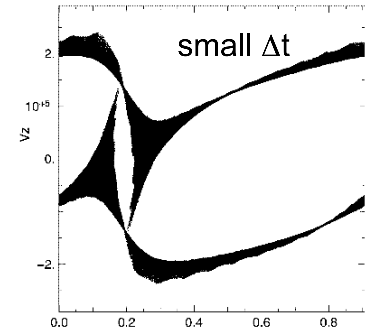
Test problem: Two-stream instability of finite-size beams (one of many tests done)

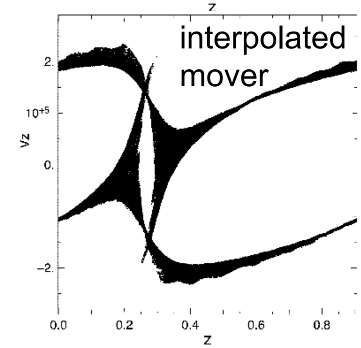


- Uniform B field
- Counter-streaming proton beams, 10 ρ_i across
- $\omega_c/\omega_p = 48$; $v_b/v_{th} = 0.1$; $L/\rho_i \approx 60$
- Compare: small Δt ($\omega_c \Delta t = 0.6$), large δt ($\omega_c \Delta t = 12$) with interpolation; large Δt with Boris mover (Parker-Birdsall)
- Finite beam-size effect: comparison with 20 ρ_i beam



- Red (large-Δt, blended) and black (small-Δt) agree well
- Blue (large- Δt Boris) fails to show instability.
- Gray (blended, 20-ρ_i beam instead of 10) has different growth rate, illustrating effect of finite beam size.
- Detailed phase-space snapshots almost identical



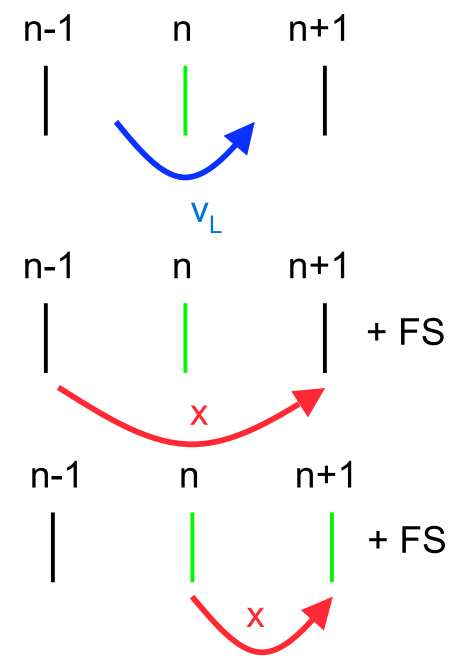


We are moving to implicitness to handle higher densities

- We would like to apply the mover to higher-density problems where the plasma frequency > cyclotron frequency.
  – e.g., neutralized drift compression, plasma instabilities,…
- First steps reported at last HIF Symposium:
  (Ref.: R. Cohen et al, NIM A **577**, 52 (2007))
  – Full centered predictor-corrector
  – Use average drift (vs drift at average position) in corrector
  – field solve after predictor & corrector
  – Polarization drift added into Poisson equation

$$\nabla^2\phi + \sum_s \nabla_\perp\left((1-\alpha)^2\omega_{ps}^2/\omega_{cs}^2\right)\nabla_\perp\phi = -4\pi e(n_i - n_e)$$

  - Adds some implicitness (perpendicular dynamics)



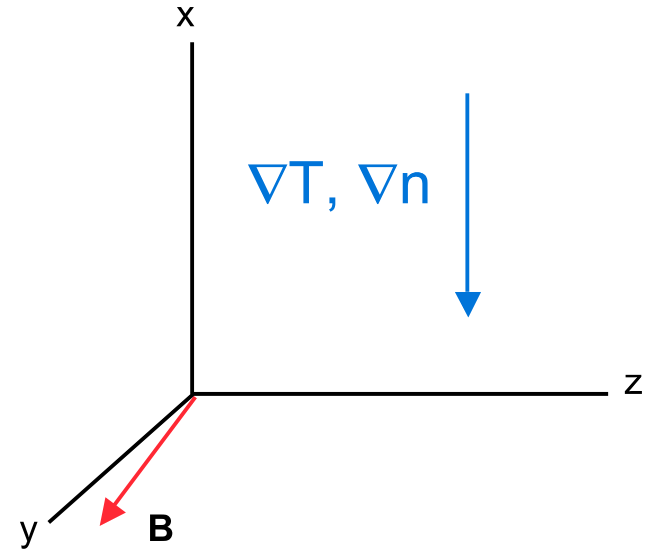
A test problem from magnetized plasma physics illustrates capability of upgraded mover

- "Ion temperature-gradient" instability in a uniform B field
  - Unstable when $\nabla_\perp \ln T \gtrsim 2\, \nabla_\perp \ln n$
  - A classic elementary test problem for MFE gyrokinetic codes
  - Simulate in 2D, x-z
  - Use multiscale trick developed in GK community: simulate effect of gradients by adding fake drift to x advance in a uniform-plasma simulation,

$$\Delta \mathbf{v} = \left(\kappa_n - (3/2 - v^2/v_{th}^2)\kappa_T\right)\mathbf{e}_x \times \mathbf{B}\,\Phi/B$$

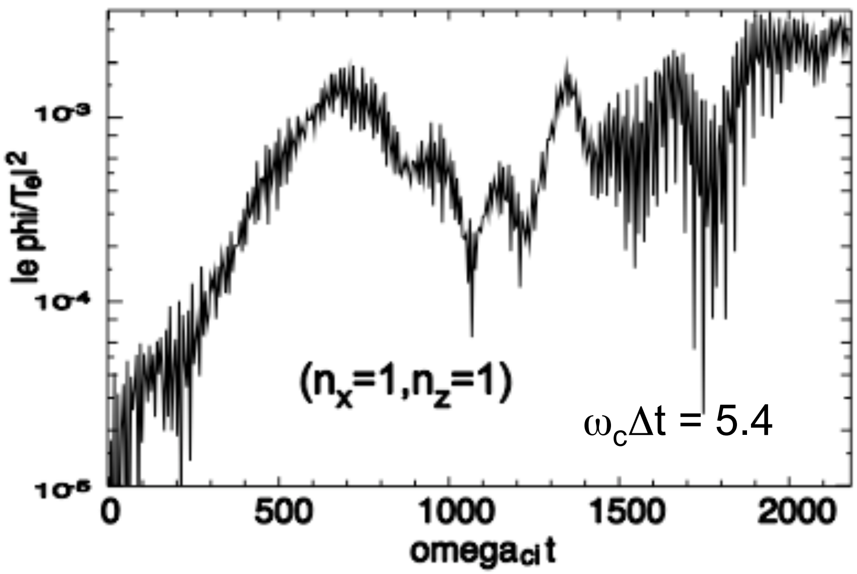
where

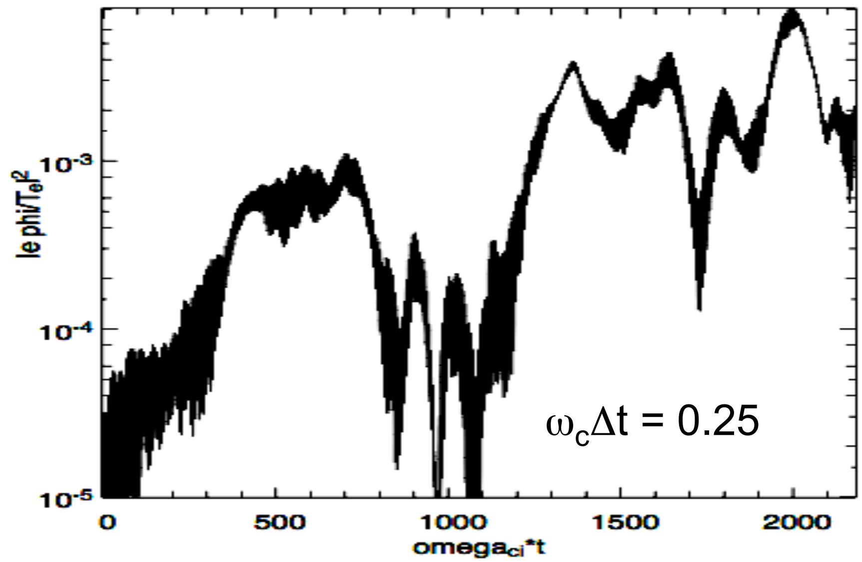
$$\kappa_n = -(1/n)dn/dx \text{ and } \kappa_T = -(1/T)dT/dx$$



  - Use adiabatic electron model, $n_e = n_0 \exp(e\Phi/T_e)$

Results for ITG test problem indicate success





- Small-timestep case noisier, hard to compare linear growth, but roughly agrees as does saturation level
- Above results are for dn/dx = 0; also good results for finite dn/dx
- Boris mover and older version of blended mover at large timestep: unstable (large amplitude fluctuations grow even with no gradients)
- Limitations:
  - 2 corrector steps required for convergence
  - Won't be adequate for more general geometry that allows modes purely || to B (this is excluded by the 2D geometry used for the present test)

A fully implicit algorithm, similar to standard PIC direct implicit, has been formulated

- In update of instantaneous velocity v_L replace E_n by $(E_{n-1}+E_{n+1})/2$
- For v_{eff} use average drift $v_d = (v_{d,n}+v_{d,n+1})/2$
- Predictor step:
  - Separate predicted $x_{n+1} = \tilde{x}_{n+1}+\delta x$, with $\tilde{x}_{n+1}$ obtained setting $E_{n+1} = 0$ in evaluation of v_L and v_d.
  - Calculate charge density due to δx (linearized in E_{n+1} at positions $\tilde{x}_{n+1}$, including polarization), and bring to left-hand side of Poisson equation:

    $$\nabla\cdot\left(\mathbf{I}+\chi\right)\cdot\nabla\phi = -4\pi\rho \quad \text{with}$$

    $$\chi = \sum \frac{\omega_p^2 \Delta t^2}{2}\left(\alpha\mathbf{T}+(1-\alpha)\mathbf{bb}\right)+\frac{\omega_p^2}{\omega_c^2}(1-\alpha)^2(\mathbf{I}-\mathbf{bb})-\frac{\omega_p^2\Delta t}{2\omega_c B}(1-\alpha)\mathbf{b}\times\mathbf{I}$$

    and T = Birdsall-Langdon rotation tensor
  - Perform field solve
- Corrector step:
  - Recalculate x_{n+1} including the δx contributions

Some remarks on this procedure

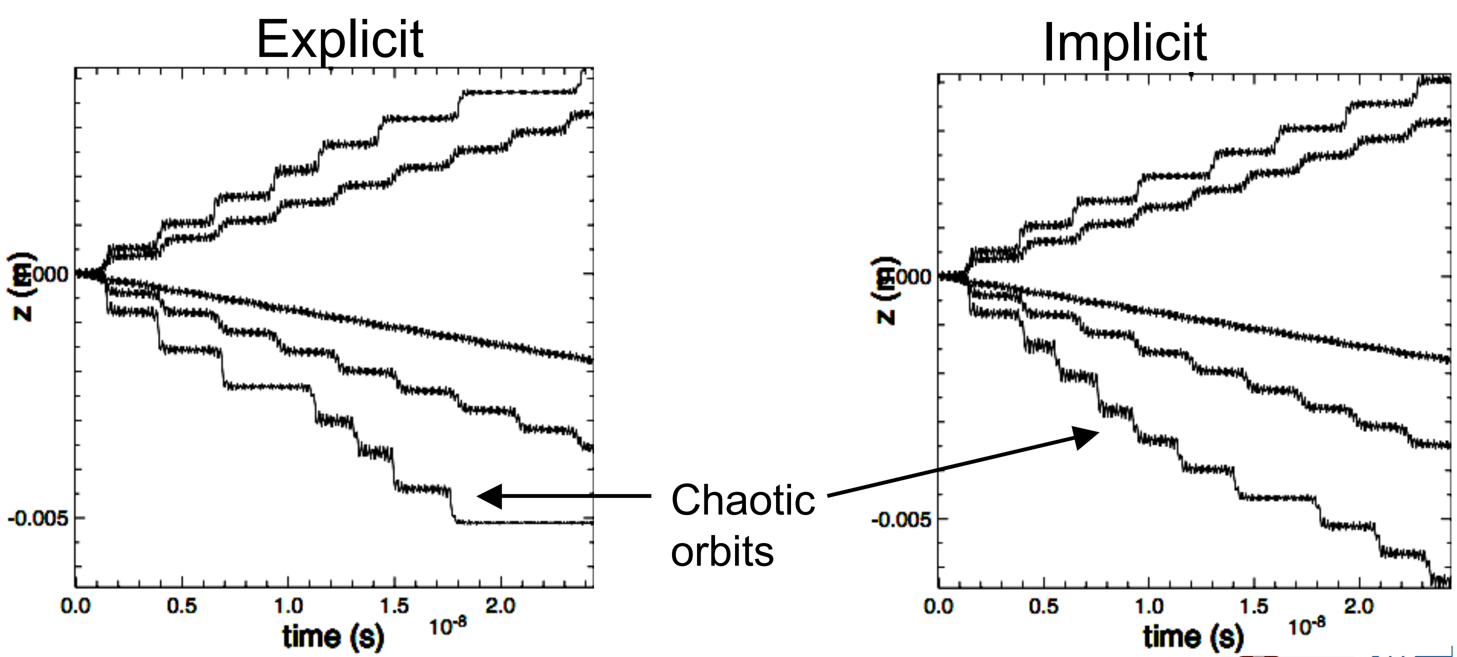
- It is implicit in drifts as well as Lorentz part
  - The contribution to field equation from ExB drift survives because $\alpha_i \neq \alpha_e$ (in contrast to pure drift kinetics)
- Only one field solve per timestep (so actually faster than procedure reported at HIF06)
- As with full-dynamics implicit, the large effective susceptibility suppresses noise in field solve
- An alternative approach is to leave the drifts fully explicit (except for polarization). This is simpler to formulate, and applicable to pure drift kinetics. But it would likely require the leapfrog predictor corrector described earlier (including the extra field solve) for stability. We haven't analyzed this but will if there is a reason to do so.

Stability analysis of intermediate and fully implicit schemes show promise of the new scheme

- Stability analysis for older scheme (polarization + predictor-corrector) indicates instability for single corrector step
  - Take cold-plasma limit of equations for uniform plasma, x-z geometry, with field in x-y plane (as in ITG test problem); adiabatic electrons.
  - Consistent with observation that we need two correctors, and have a residual period-2 oscillation
- Corresponding analysis for fully implicit scheme indicates only stable roots.

Tests: single particle orbits

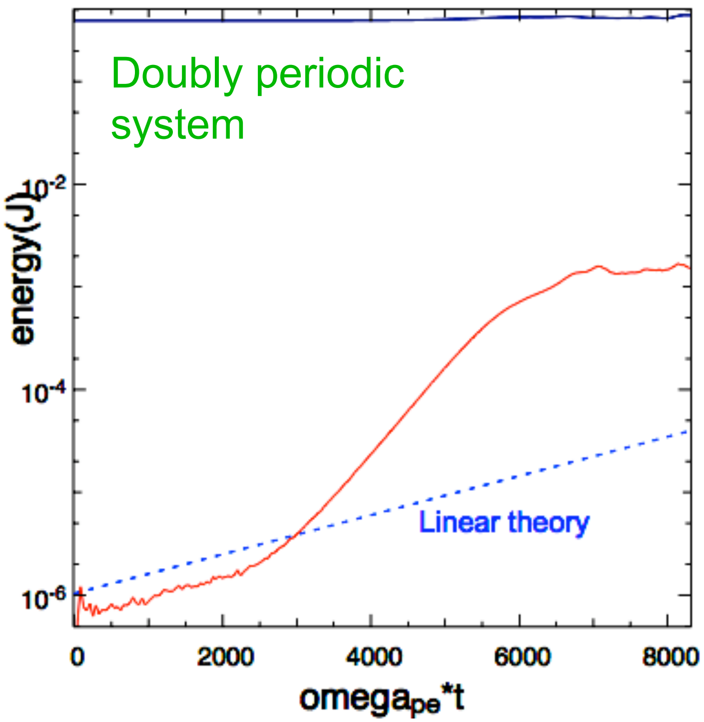
- Algorithm has been implemented in WARP
- Particle-mover tests look great
  - Examine electron particle orbits which pass near null of magnetic quadrupole with fixed large positive charge (representing an ion beam) in central region
  - Compare explicit and implicit DL movers for $\omega_{ce}\Delta t \approx 16$ (previously showed excellent agreement of explicit results with small-timestep full-ion dynamics)

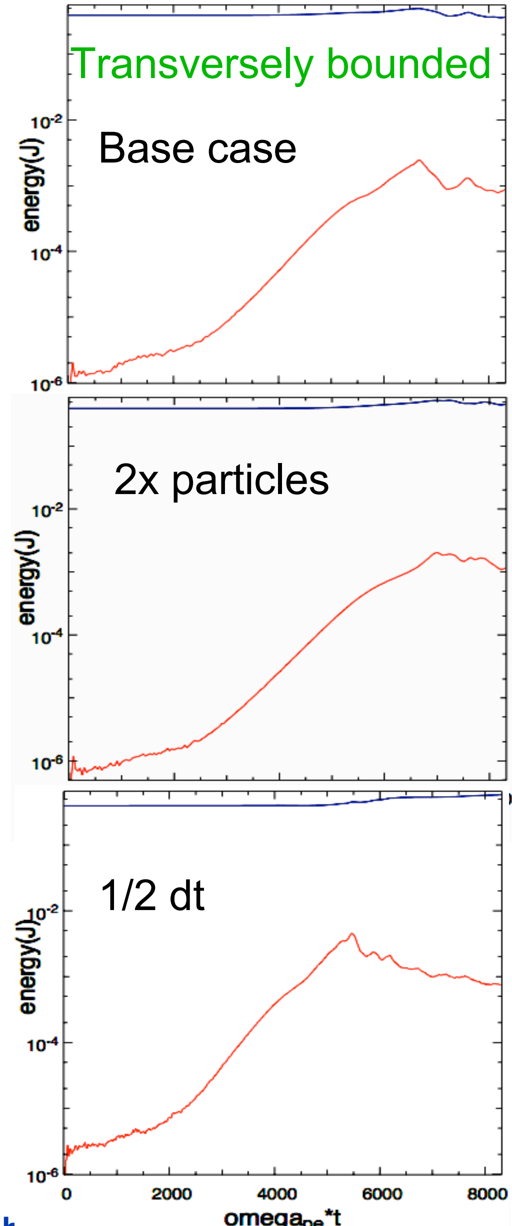


Tests: Buneman Instability in a uniform B field

- Buneman instability = two-stream instability of electrons drifting through ions
  – Growth rate ~ $(m/M)^{1/3}\ \omega_{pe}$ $\Rightarrow$can pick $\omega_{pe}\Delta t \sim \omega_{ce}\Delta t > 1$ to test implicitness
- Adding uniform B along drift direction:
  – In infinite plasma (or one with periodic transverse b.c.'s), doesn't change dispersion relation -- can compare with 1D analytic theory
  – In bounded plasma (Dirichlet conditions on potential in transverse directions), perpendicular dynamics matters, finite gyroradius plays a role.
- Test cases:
  – x-z geometry, B in z direction, particles and fields periodic in z
  – Particles and fields periodic or reflecting/Dirichlet in x.
  – $\omega_{pe}/\omega_{ce} = 4$; x domain = 40 gyro diameters; z domain = 201 in units of $(M/m)^{1/3}\ \lambda_{Debye.}$
  – Results:

Buneman results





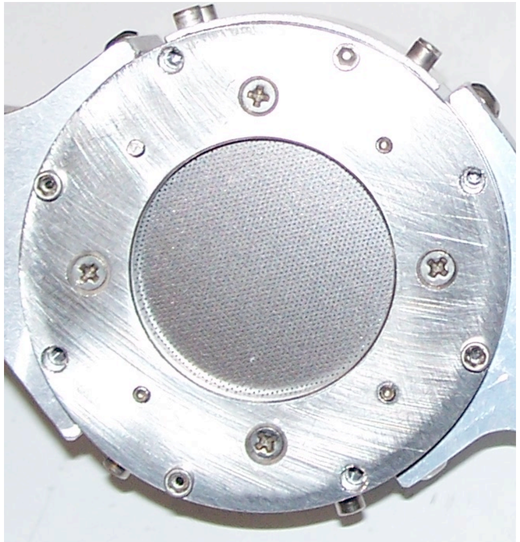
- No instability for zero relative drift
- Full-dynamics implicit and expliciit cases numerically unstable (with no relative v)
- Super-linear phase growth shared by all harmonics.

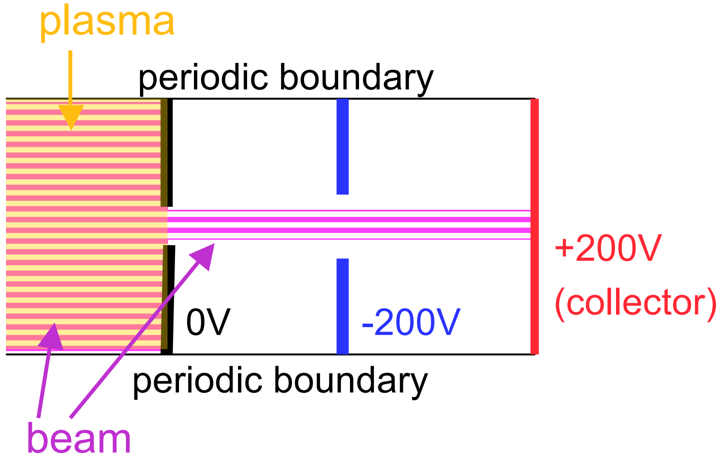
Buneman -- summary of results: Scheme is reasonably accurate and needed for large-dt stability

- For periodic B.C.'s implicit code's initial growth matches well to linear theory (and shows in 10's of steps).
  - Subsequent super-linear growth observed in all Fourier modes; nonlinear instability?
  - Implicit solution without drift-Lorentz interpolation the solution is UNSTABLE (even with no e-i relative drift).
  - Explicit with same long timestep solution is UNSTABLE.
  - Explicit solution with resolved ω_{pe} (45x smaller timestep) is stable but too noisy to see linear growth (even for 10x more particles).
- For bounded transverse BC's, no longer textbook theory -- but results have reasonable convergence with respect to resolution, particle number.

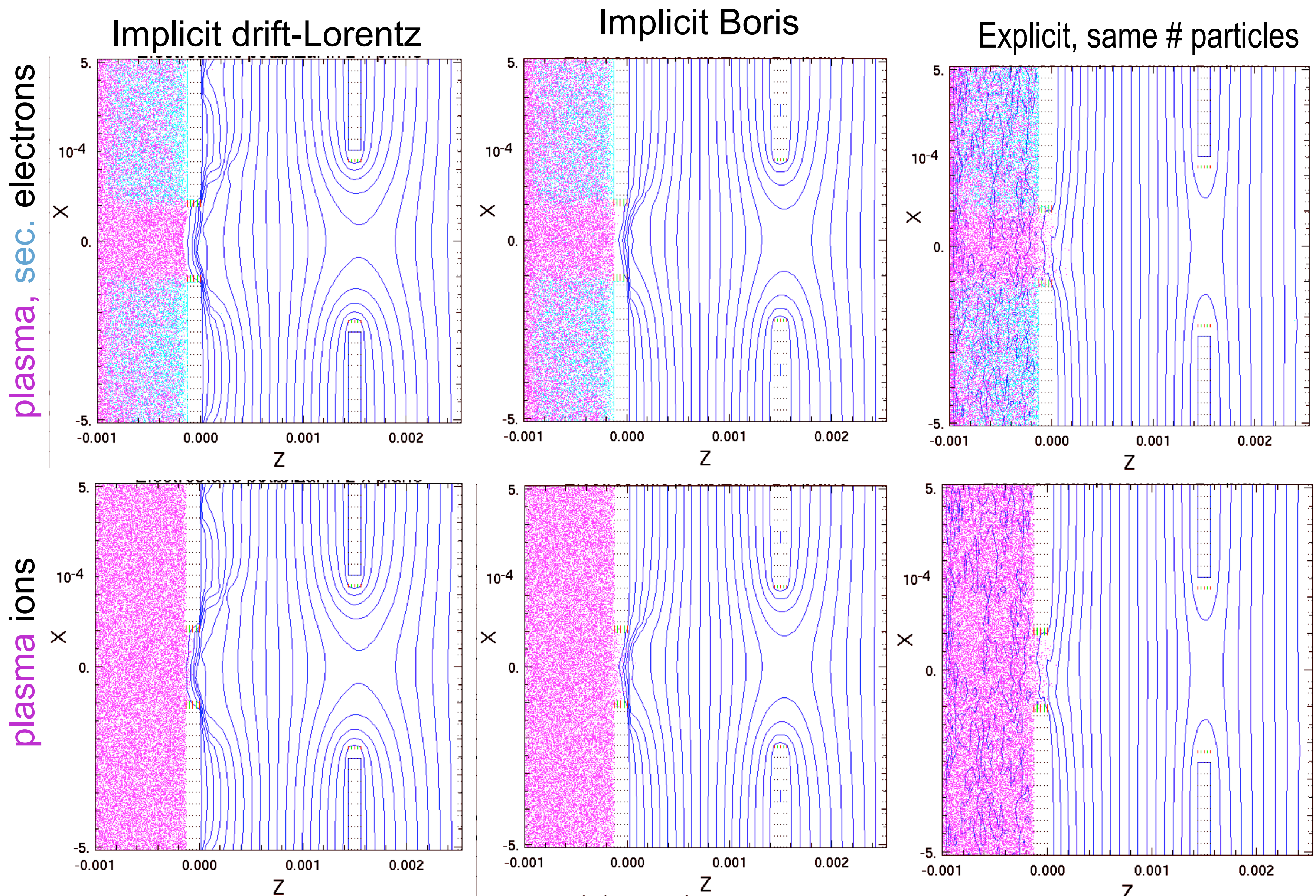
Fast Faraday Cup (FFC) presents a test problem of practical interest for HIF/HEDP

- The FFC was devised to measure ion beam current in the presence of neutralizing plasma
  - Front and midplates with small holes to exclude plasma from reaching collector plate
  - Modeling challenge: want to follow gas buildup/ionization on timescales ~ μs; must follow beam transit times ~ ns; would like to avoid resolving electron cyclotron and plasma frequencies ~ 10^{-11} s.
  - Verification test here: show that we can with accuracy beat the ω_{pe},ω_{ce} time restrictions.





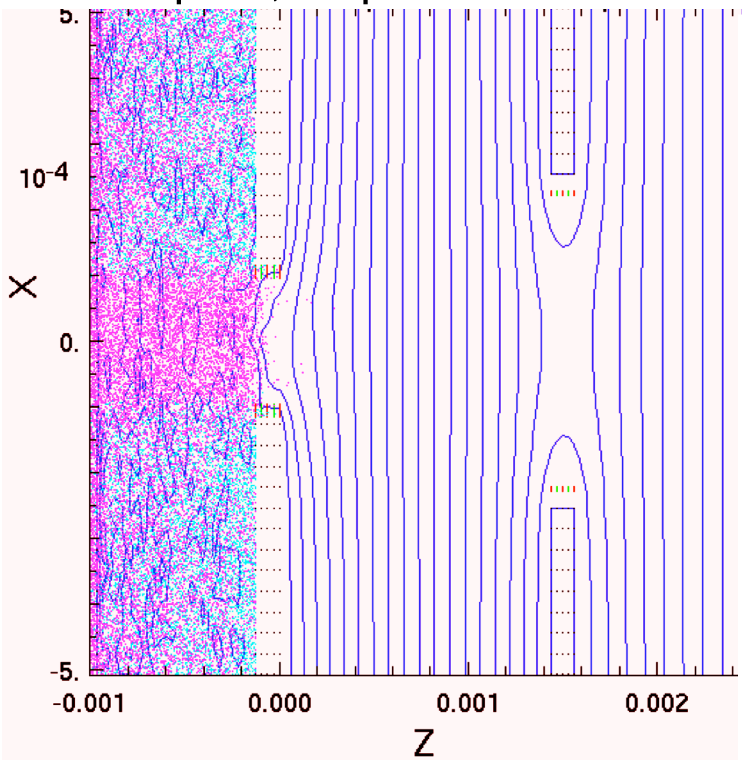
Implicit $\omega_{pe}\Delta t$=12 simulations reproduce well explicit simulations with 20x more steps and 10x more particles



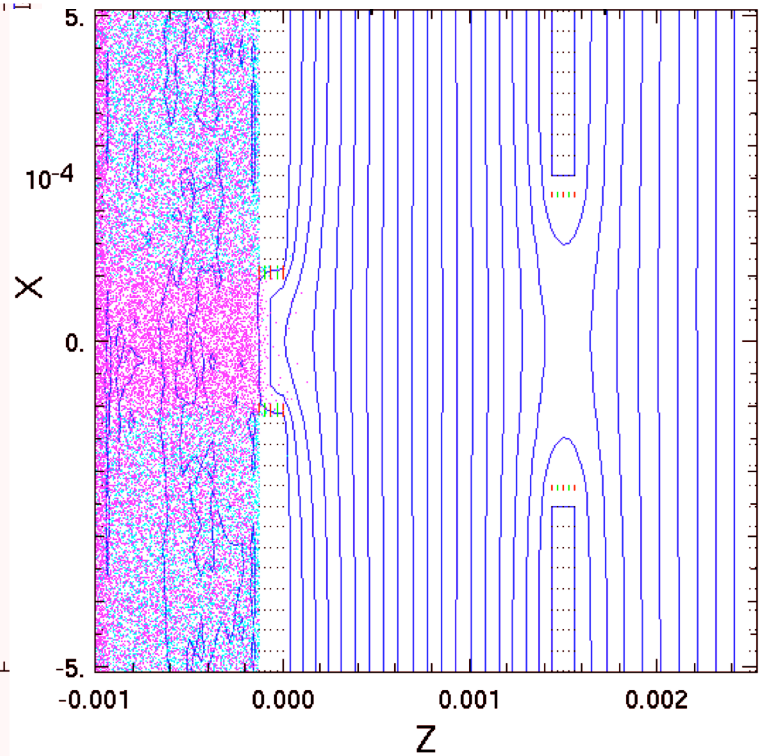
Residual differences with explicit appear to be result of noise in explicit, reduced by 10x more particles

- Compare runs where affordable (1/2 way through):

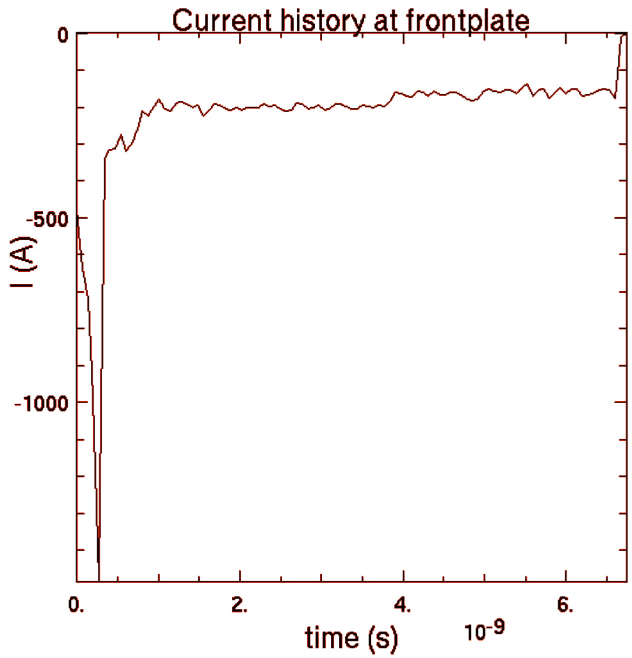
Explicit, 1x particles

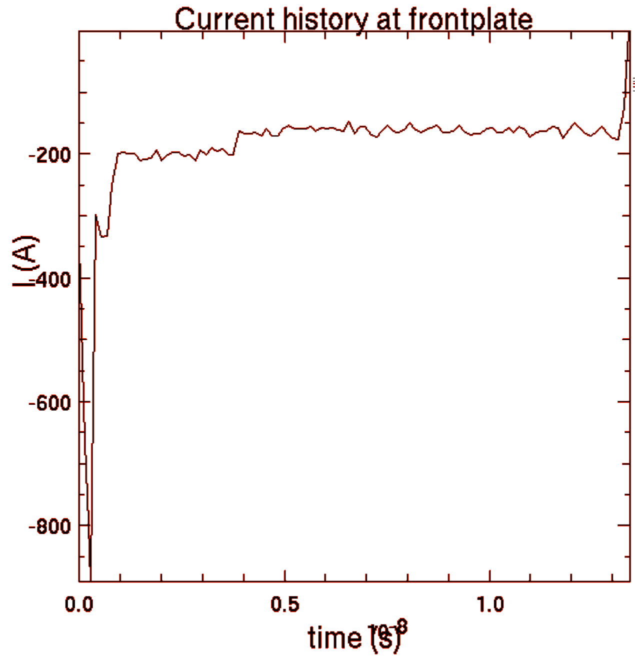


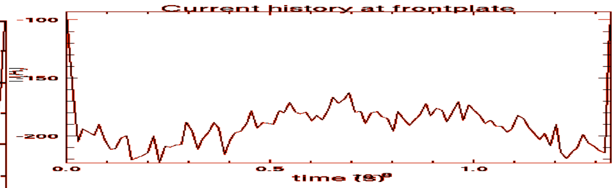
Explicit, 10x particles



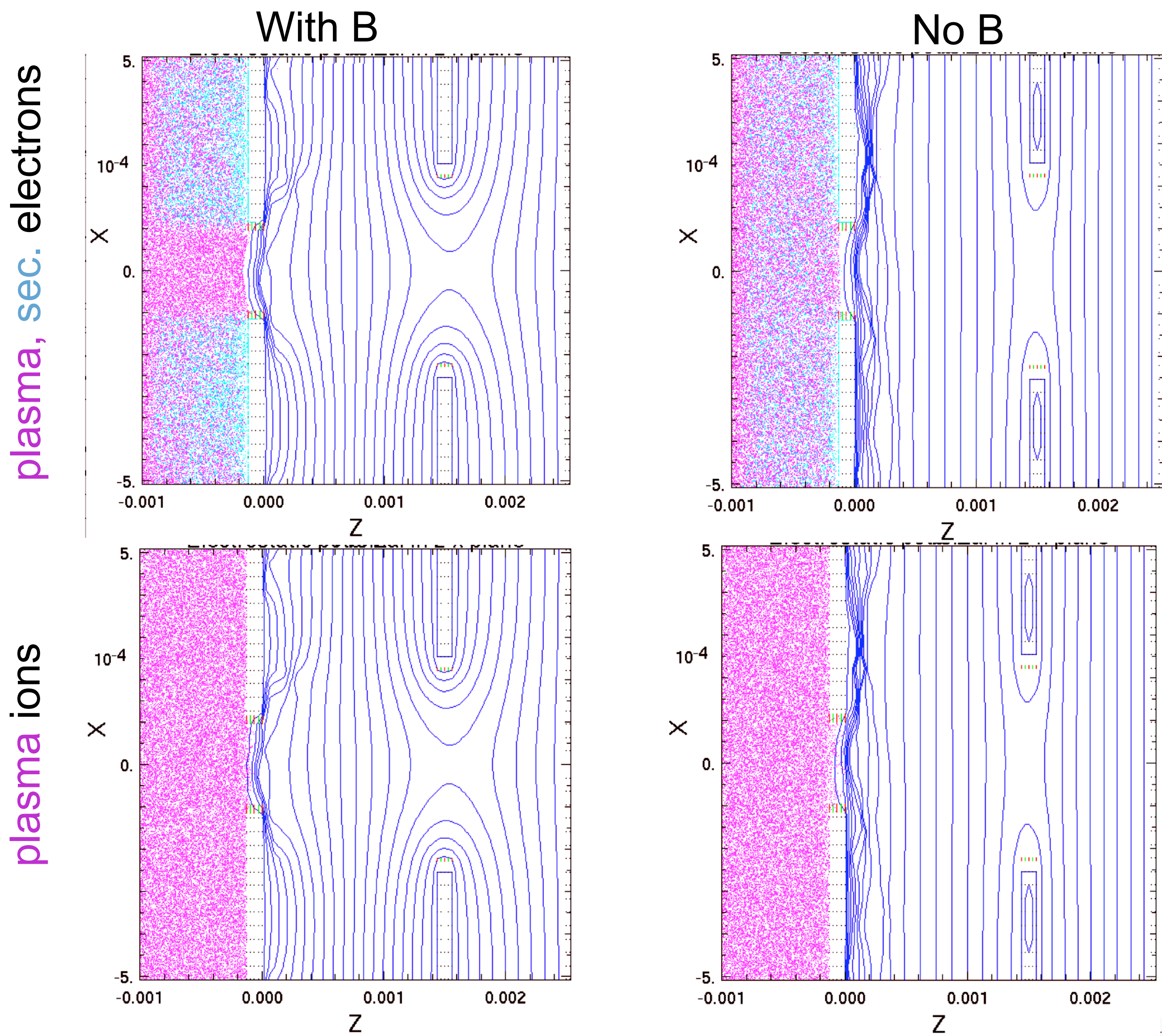
Current histories agree apart from initial spike



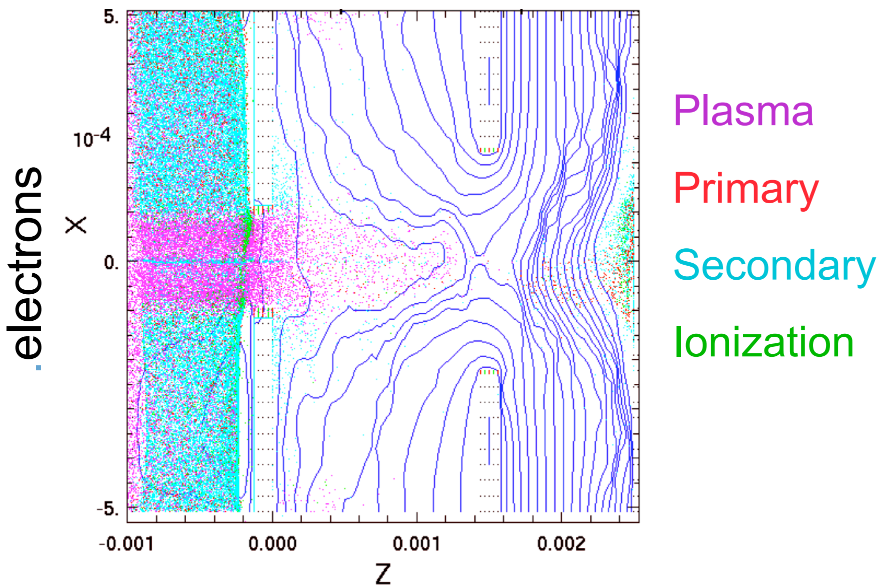


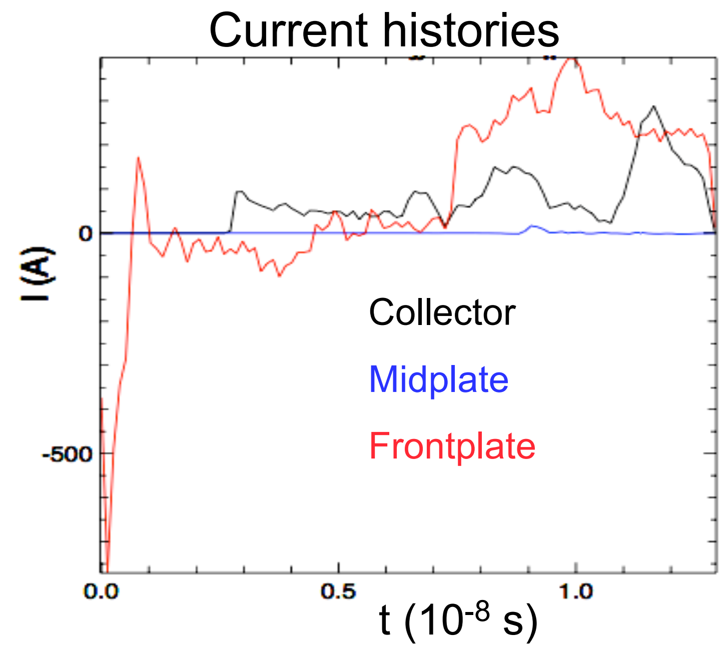


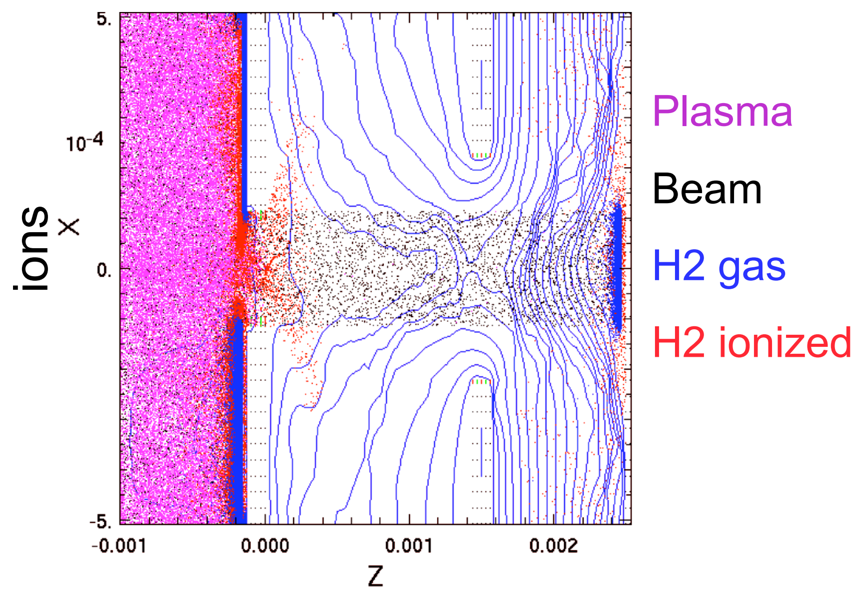
Effect of B field is small -- mainly affects where secondaries go



We have obtained our first "full-physics" FFC results, including beams, gas transport, ionization (still early time)







Summary of FFC test

- Implicit simulation $\omega_{pe}\Delta t>1$, $\omega_{ce}\Delta t>1$ works (stable, accurate) for either drift-Lorentz or straight Boris scheme
  – But beware, Buneman test showed straight Boris unstable in this regime for parameters not very different from these.
- Residual difference with explicit case plausibly due to increased noise in explicit field solve; need more particles in addition to smaller timestep for accurate explicit solve.
- Effect of B field on plasma is weak; mainly impacts secondary electron distribution
- We are now working on “full-physics runs” with beam propagation, gas and electron desorption, gas propagation, and ionization.

Why implicit drift-Lorentz versus implicit with full (Boris) ion dynamics at large $\omega_{pe}\delta t$, $\omega_{ce}\delta t$

- For accuracy and energy conservation, want to run implicit simulations with $v_{th}\ \delta t/\ \delta z \sim 1$.
  - For large $\omega_{ce}\delta t$, the effective gyro diameter for Boris is $v_{th}\ \delta t > \rho$.
  - For simulations with cells elongated in z (along B), drift-Lorentz is preferred because of accuracy: a likely problem with Boris since effective gyro diameter can be many radial cells.
  - The other advantage is stability; we've shown by example that pure Boris can be unstable, even for square cells.

Summary

- Blended “drift-Lorentz mover” allows efficient treatment of particle orbits in strong and weak (or no) magnetic fields.
- Extension to include polarization drift in field solve introduces some implicitness; demonstrated via solution of slab ion-temperature gradient instability
  – Requires two corrector steps; new stability analysis indicates why (single corrector unstable with odd-even instability, as observed).
- An implicit algorithm -- analogy of direct implicit approach -- has been developed for the drift-Lorentz mover. Stability analysis indicates large-timestep stability.
  – Successful verification results for particle orbit, Buneman, fast-faraday cup (FFC) test problems.
  – Buneman test problem demonstrates that implicit drift-Lorentz can provide stability where conventional implicit + Boris mover would be unstable.
  – Accuracy advantage for cells elongated along B.
- FFC results indicate weak affect of applied B field
- Turning attention now to FFC runs with “full physics”

BACKUP SLIDES

Stability analysis for older scheme (polarization + predictor-corrector) indicates instability for single corrector step

- Take cold-plasma limit of equations for uniform plasma, x-z geometry, with field in x-y plane (as in ITG test problem); adiabatic electrons.
- Assume $x^{(n)} \sim X\lambda^n$; find dispersion relation in terms of λ.
- For the predictor-corrector mover with polarization and $2\Delta t$ predictor, and a single corrector step, we find, for large timesteps, a pair of coupled equations in the amplitudes X and Z:

$$\frac{\alpha}{2}\frac{2cb_yX + \left(4 + b_z^2c^2\right)Z}{(4+c^2)} + (1-\alpha^2)^2\frac{\omega_p^2}{\omega_c^2}b_y^2 + (1-\alpha)b_z^2/2 = 0$$

$$\alpha\frac{2X - cb_yZ}{4+c^2} - (1-\alpha^2)^2\frac{\omega_p^2}{\omega_c^2}(X - b_zb_yZ) + b_zb_yZ/2 = 0$$

with $c = (\omega_c\Delta t/2)(1+1/\lambda)$; $b_y=B_y/B$, etc; quadratic disp. rel. in c^2

  – For large $\omega_c\Delta t$ there is always a root with $\lambda \sim -1 - \varepsilon$, unstable and oscillating. Consistent with observation that we need two correctors, and have a residual period-2 oscillation

Stability analysis for new implicit algorithm indicates large-timestep stability

- For implicit scheme the analagous coupled equations are (limit of large $\theta = \omega_c \Delta t/2$ and large $\omega_p \Delta t$):

$$\frac{\lambda+1}{\lambda-1}X - \frac{b_y Z}{\theta} = 0$$

$$\frac{\alpha b_y X}{\theta} + \left(\alpha + \frac{2\lambda b_z^2}{\lambda-1}\right) Z = 0$$

- This has two roots, both stable:

$$\lambda \approx 1/(1+2b_z^2/\alpha) \quad \text{and} \quad \lambda \approx -1 + \frac{2\alpha b_y^2}{\theta^2(\alpha + b_z^2)}$$